

A Primer on Resonances in Quantum Mechanics

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Abstract

After a pedagogical introduction to the concept of resonance in classical and quantum mechanics, some interesting applications are discussed. The subject includes resonances occurring as one of the effects of radiative reaction, the resonances involved in the refraction of electromagnetic waves by a medium with a complex refractive index, and quantum decaying systems described in terms of resonant states of the energy. Some useful mathematical approaches like the Fourier transform, the complex scaling method and the Darboux transformation are also reviewed.

1 Introduction

Solutions of the Schrödinger equation associated to complex eigenvalues $\epsilon = E - i\Gamma/2$ and satisfying purely outgoing conditions are known as Gamow-Siegert functions [1, 2]. These solutions represent a special case of scattering states for which the ‘capture’ of the incident wave produces delays in the scattered wave. The ‘time of capture’ can be connected with the lifetime of a decaying system (resonance state) which is composed by the scatterer and the incident wave. Then, it is usual to take $\text{Re}(\epsilon)$ as the binding energy of the composite while $\text{Im}(\epsilon)$ corresponds to the inverse of its lifetime. The Gamow-Siegert functions are not admissible as physical solutions into the mathematical structure of Quantum Mechanics since, in contrast with conventional scattering wave-functions, they are not finite at $r \rightarrow \infty$. Thus, such a kind of functions is acceptable in Quantum Mechanics only as a convenient model to solve scattering equations. However, because of the resonance states relevance, some approaches extend the formalism of quantum theory so that they can be defined in a precise form [3–8].

The concept of resonance arises from the study of oscillating systems in classical mechanics and extends its applications to physical theories like electromagnetism, optics, acoustics, and quantum mechanics, among others. In this context, resonance may be defined as the excitation of a system by matching the frequency of an applied force to a characteristic frequency of the system. Among the big quantity of examples of resonance in daily life one can include the motion of a child in a swing or the tuning of a radio or a television receiver. In the former case you must push the swing from time to time to maintain constant the amplitude of the oscillation. In case you want to increase the amplitude you should push ‘with the natural motion’ of the swing. That is, the acting of the force you are applying on the swing should be in ‘resonance’ with the swing motion. On the other hand, among the extremely large number of electromagnetic signals in space,

your radio responds only to that one for which it is tuned. In other words, the set has to be in resonance with a specific electromagnetic wave to permit subsequent amplification to an audible level. In this paper we present some basics of resonance phenomenon. It is our intent to provide a strong primer introduction to the subject rather than a complete treatment. In the next sections we shall discuss classical models of vibrating systems giving rise to resonance states of the energy. Then we shall review some results arising from the Fourier transform widely used in optics and quantum mechanics. This material will be useful in the discussions on the effects of radiative reaction which are of great importance in the study of atomic systems. We leave for the second part of these notes the discussion on the resonances in quantum decaying systems and their similitudes with the behavior of optical devices including a complex refractive index. Then the complex scaling method arising in theories like physical chemistry is briefly reviewed to finish with a novel application of the ancient Darboux transformation in which the transformation function is a quantum resonant state of the energy. At the very end of the paper some lines are included as conclusions.

2 Vibration, Waves and Resonances

2.1 Mechanical Models

Ideal vibrating (or oscillating) systems undergo the same motion over and over again. A very simple model consists of a mass m at the end of a spring which can slide back and forth without friction. The time taken to make a complete vibration is the *period* of oscillation while the *frequency* is the number of vibration cycles completed by the system in unit time. The motion is governed by the acceleration of the vibrating mass

$$\frac{d^2x}{dt^2} = -\left(\frac{k}{m}\right)x \equiv -w_0^2x \quad (1)$$

where $w_0 := \sqrt{k/m}$ is the *natural angular frequency* of the system. In other words, a general displacement of the mass follows the rule

$$x = A \cos w_0 t + B \sin w_0 t \quad (2)$$

with A and B two arbitrary constants. To simplify our analysis we shall consider a particular solution by taking $A = a \cos \theta$ and $B = -a \sin \theta$, therefore we can write

$$x = a \cos(w_0 t + \theta). \quad (3)$$

At $t_n = \frac{(2n+1)\pi - \theta}{2w_0}$, $n = 0, 1, 2, \dots$, the kinetic energy $T = \frac{1}{2}m(dx/dt)^2$ reaches its maximum value $T_{\max} = mw_0^2 a^2/2$ while x passes through zero. On the other hand, the kinetic energy is zero and the displacement of the mass is maximum ($x = a$ is the *amplitude* of the oscillation) at $t_m = \frac{m\pi - \theta}{w_0}$, $m = 0, 1, 2, \dots$. This variation of T is just opposite of that of the potential energy $V = kx^2/2$. As a consequence, the total stored energy E

is a constant of motion which is proportional to the square of the amplitude (twice the amplitude means an oscillation which has four times the energy):

$$E = T + V = \frac{1}{2}mw_0^2a^2. \quad (4)$$

Systems exhibiting such behavior are known as *harmonic oscillators*. There are plenty of examples: a weight on a spring, a pendulum with small swing, acoustical devices producing sound, the oscillations of charge flowing back and forth in an electrical circuit, the ‘vibrations’ of electrons in an atom producing light waves, the electrical and magnetical components of electromagnetic waves, and so on.

2.1.1 Steady-state oscillations

In actual vibrating systems there is some loss of energy due to friction forces. In other words, the amplitude of their oscillations is a decreasing function of time (the vibration *damps down*) and we say the system is *damped*. This situation occurs, for example, when the oscillator is immersed in a viscous medium like air, oil or water. In a first approach the friction force is proportional to the velocity $F_f = -\alpha \frac{dx}{dt}$, with α a *damping constant* expressed in units of mass times frequency. Hence, external energy must be supplied into the system to avoid the damping down of oscillations. In general, vibrations can be driven by a repetitive force $F(t)$ acting on the oscillator. So long as $F(t)$ is acting there is an amount of work done to maintain the stored energy (i.e., to keep constant the amplitude). Next we shall discuss the forced oscillator with damping for a natural frequency w_0 and a damping constant α given.

Let us consider an oscillating force defined as the real part of $F(t) = Fe^{iwt} \equiv F_0e^{i(wt+\eta)}$. Our problem is to solve the equation

$$\frac{d^2x}{dt^2} + \gamma \frac{dx}{dt} + w_0^2x = \text{Re} \left(\frac{Fe^{iwt}}{m} \right), \quad \gamma := \frac{\alpha}{m}. \quad (5)$$

Here the new damping constant γ is expressed in units of frequency. The ansatz $x = \text{Re}(ze^{iwt})$ reduces (5) to a factorizable expression of z , from which we get

$$z = \frac{F\Omega}{m}, \quad \Omega = \frac{1}{w_0^2 - w^2 + i\gamma w}. \quad (6)$$

We realize that z is proportional to the complex function Ω , depending on the driving force’s frequency w and parameterized by the natural frequency w_0 and the damping constant γ . In polar form $\Omega = |\Omega|e^{i\phi}$, the involved phase angle ϕ is easily calculated by noticing that $\Omega^{-1} = e^{-i\phi}/|\Omega| = w_0^2 - w^2 + i\gamma w$, so we get

$$\tan \phi = -\frac{\gamma w}{w_0^2 - w^2}. \quad (7)$$

Let us construct a single valued phase angle ϕ for finite values of w_0 and γ . Notice that $w < w_0$ leads to $\tan \phi < 0$ while $w \rightarrow w_0^-$ implies $\tan \phi \rightarrow -\infty$. Thereby we can set

$\phi(w = 0) = 0$ and $\phi(w_0) = -\pi/2$ to get $\phi \in [-\pi/2, 0]$ for $w \leq w_0$. Now, since $w > w_0$ produces $\tan \phi > 0$, we use $\tan(-\phi) = -\tan \phi$ to extend the above defined domain $\phi \in (-\pi, 0]$, no matter the value of the angular frequency w . Bearing these results in mind we calculate the real part of z (see equation 6) to get the physical solution

$$x = x_0 \cos(wt + \eta + \phi), \quad x_0 := \frac{F_0 |\Omega|}{m}. \quad (8)$$

Notice that the mass oscillation is not in phase with the driving force but is shifted by ϕ . Moreover, $\gamma \rightarrow 0$ produces $\phi \rightarrow 0$, so that this phase shift is a measure of the damping. Since the phase angle is always negative or zero ($-\pi/2 < \phi \leq 0$), equation (8) also means that the displacement x lags behind the force $F(t)$ by an amount ϕ . On the other hand, the amplitude x_0 results from the quotient F_0/m scaled up by $|\Omega|$. Thus, such a scale factor gives us a measure of the response of the oscillator to the action of the driving force. The total energy (4), with $a = x_0$, is then a function of the angular frequency:

$$E(w) = \frac{(w_0 F_0)^2}{2m} |\Omega|^2 \equiv \frac{(w_0 F_0)^2}{2m} \left[\frac{1}{(w_0^2 - w^2)^2 + (\gamma w)^2} \right]. \quad (9)$$

Equations (7) and (9) comprise the complete solution to the problem. The last one, in particular, represents the *spectral energy distribution* of the forced oscillator with damping we are dealing with. It is useful, however, to simplify further under the assumption that $\gamma \ll 1$. For values of w closer to that of w_0 the energy approaches its maximum value $2mE(w_0) \approx (F_0/\gamma)^2$ while $E(w \rightarrow +\infty)$ goes to zero as w^{-4} . In other words, $E(w)$ shows rapid variations only near w_0 . It is then reasonable to substitute

$$w_0^2 - w^2 = (w_0 - w)(w_0 + w) \approx (w_0 - w)2w_0 \quad (10)$$

in the expressions of the energy and the phase shift to get

$$E(w \rightarrow w_0) \approx \frac{1}{2m} \left(\frac{F_0}{\gamma} \right)^2 \omega(w, w_0, \gamma), \quad \tan \phi \approx \frac{\gamma}{2(w - w_0)} \quad (11)$$

with

$$\omega(w, w_0, \gamma) := \frac{(\gamma/2)^2}{(w_0 - w)^2 + (\gamma/2)^2}. \quad (12)$$

Equation (12) describes a bell-shaped curve known as the *Cauchy* (mathematics), *Lorentz* (statistical physics) or *Fock-Breit-Wigner* (nuclear and particle physics) distribution. It is centered at $w = w_0$ (the *location parameter*), with a half-width at half-maximum equal to $\gamma/2$ (the *scale parameter*) and amplitude (height) equal to 1. That is, the damping constant γ defines the width of the spectral line between the half-maximum points $w_0 - w = \pm \gamma/2$. Fig. 1 shows the behavior of the curve ω for different values of the damping constant (*spectral width*) γ .

These last results show that the adding of energy to the damping oscillator is most efficient if the vibrations are sustained at a frequency $w = w_0$. In such a case it is said that the driving force is in *resonance* with the oscillator and w_0 is called the *resonance frequency*. Besides the above discussed spring-mass system, the motion of a child in a

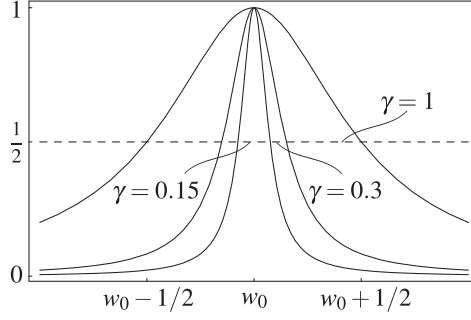


Figure 1: The Fock-Breit-Wigner (Lorentz-Cauchy) distribution ω for different values of the width at half maximum γ .

swing is another simple example giving rise to the same profile. To keep the child+swing system oscillating at constant amplitude you must push it from time to time. To increase the amplitude you should push ‘with the motion’: the oscillator vibrates most strongly when the frequency of the driving force is equal to the frequency of the free vibration of the system. On the other hand, if you push against the motion, the oscillator do work on you and the vibration can be brought to a stop. The above cases include an external force steading the oscillations of the system. This is why equations (7–9) are known as the *steady-state* solutions of the problem.

We can calculate the amount of work W_{work} which is done by the driving force. This can be measured in terms of the *power* P , which is the work done by the force per unit time:

$$P = \frac{d}{dt}W_{\text{work}} = F(t)\frac{dx}{dt} = \frac{dE}{dt} + m\gamma \left(\frac{dx}{dt}\right)^2. \quad (13)$$

The *average* power $\langle P \rangle$ corresponds to the *mean* of P over many cycles. To calculate it we first notice that $\langle dE/dt \rangle = 0$. That is, the energy E does not change over a period of time much larger than the period of oscillation. Now, since the square of any sinusoidal function has an average equal to $1/2$, the last term in (13) has an average which is proportional to the square of the frequency times the amplitude of the oscillation. From (8) we get

$$\langle P \rangle = \frac{m\gamma w^2 x_0^2}{2}. \quad (14)$$

It is then clear that the driving force does a great deal of work to cancel the action of the friction force. In a similar form we obtain the average of the stored energy:

$$\langle E \rangle = \frac{mx_0^2(w^2 + w_0^2)}{4}. \quad (15)$$

Remark that the mean of E does not depend on the friction but on the angular frequency of the driving force. If w is close to the resonance frequency w_0 , then $\langle E \rangle$ goes to the ideal oscillator’s energy (4), scaled by $(x_0/a)^2$. Moreover, the same result is obtained no matter the magnitude of the driving force, since it does not play any role in (15).

2.1.2 Transient oscillations

Suppose a situation in which the driving force is turned off at a given time $t = t_0$. This means no work is done to sustain the oscillations so that there is no supplied energy to preserve the motion any longer. This system can be studied by solving (5) with $F = 0$. After introducing the ansatz $x = \text{Re}(ze^{i\omega t})$ we get a quadratic equation for w , the solution of which reads

$$w_{\pm} = i\gamma/2 \pm \vartheta, \quad \vartheta := \sqrt{w_0^2 - (\gamma/2)^2}. \quad (16)$$

If $\gamma < w_0$ then $\vartheta \in \mathbf{R}$ and any of these two roots produces the desired solution:

$$x = \text{Re}(ze^{i\omega t}) = |z|e^{-\frac{\gamma}{2}t} \cos(\vartheta t + z_0), \quad t \geq t_0. \quad (17)$$

First, notice that the energy is not a constant of motion but decreases in exponential form $E \propto |z|^2 e^{-\gamma t}$. The damping constant γ is then a measure of the lifetime of the oscillation because at the time $\tau = 1/\gamma$, the energy is reduced to approximately the 36% ($E \rightarrow E/e$) while the amplitude goes to the 60% of its initial value ($|z| \rightarrow |z|/\sqrt{e}$). Thus, the smaller the value of γ the larger the lifetime τ of the oscillation. In this way, for values of γ such that $w_0 \gg \gamma/2$, the discriminant in (16) becomes $\vartheta \approx w_0$. Thereby, the system exhibits an oscillation of frequency close to the resonance frequency w_0 . This means that large lifetimes are intimately connected with resonances for small values of the damping constant.

As we can see, the resonance phenomenon is a characteristic of vibrating systems even in absence of forces sustaining the oscillations. Solutions like (17) are known as *transient* oscillations because there is no force present which can ensure their prevalence. They are useful to describe mechanical oscillators for which the driven force has been turned off at the time $t = t_0$ or, more general, decaying systems like the electric field emitted by an atom. In general, ‘resonance’ is the tendency of a vibrating system to oscillate at maximum amplitude under certain frequencies w_n , $n = 0, 1, 2, \dots$. At these resonance frequencies even small driving forces produce large amplitude vibrations. The phenomenon occurs in all type of oscillators, from mechanical and electromagnetic systems to quantum probability waves. A resonant oscillator can produce waves oscillating at specific frequencies. Even more, this can be used to pick out a specific frequency from an arbitrary vibration containing many frequencies.

2.2 Fourier Optics Models

In this section we shall review some interesting results arising from the Fourier transform. This mathematical algorithm is useful in studying the properties of optical devices, the effects of radiative reaction on the motion of charged particles and the energy spectra of quantum systems as well. Let $\{e^{ikx}\}$ be a set of plane waves orthonormalized as follows

$$(e^{ikx}, e^{i\kappa x}) = \lim_{a \rightarrow +\infty} \int_{-a}^a e^{i(k-\kappa)x} dx = \lim_{a \rightarrow +\infty} 2 \frac{\sin(k-\kappa)a}{k-\kappa} \equiv 2\pi\delta(k-\kappa) \quad (18)$$

with $\delta(x-x_0)$ the Dirac’s delta distribution. This ‘function’ arises in many fields of study and research as representing a sharp impulse applied at x_0 to the system one is dealing

with. The response of the system is then the subject of study and is known as the *impulse response* in electrical engineering, the *spread function* in optics or the *Green's function* in mathematical-physics. Among its other peculiar properties, the Dirac function is defined in such a way that it can sift out a single ordinate in the form

$$f(x_0) = \int_{-\infty}^{\infty} \delta(x - x_0) f(x) dx. \quad (19)$$

In general, a one-dimensional function $\varphi(x)$ can be expressed as the linear combination

$$\varphi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{\varphi}(k) e^{-ikx} dk \quad (20)$$

where the coefficient of the expansion $\tilde{\varphi}(k)$ is given by the following inner product

$$\begin{aligned} (e^{-ikx}, \varphi) &= \int_{-\infty}^{+\infty} \varphi(x) e^{ikx} dx = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left[\int_{-\infty}^{+\infty} e^{i(k-\kappa)x} dx \right] \tilde{\varphi}(\kappa) d\kappa \\ &= \int_{-\infty}^{+\infty} \delta(k - \kappa) \tilde{\varphi}(\kappa) d\kappa = \tilde{\varphi}(k). \end{aligned} \quad (21)$$

If (20) is interpreted as the Fourier series of $\varphi(x)$, then the continuous index k plays the role of an *angular spatial frequency*. The coefficient $\tilde{\varphi}(k)$, in turn, is called the *Fourier transform* of $\varphi(x)$ and corresponds to the amplitude of the *spatial frequency spectrum* of $\varphi(x)$ between k and $k + dk$. It is also remarkable that functions (20) and (21) are connected via the Parseval formula

$$\int_{-\infty}^{+\infty} |\varphi(x)|^2 dx = \int_{-\infty}^{+\infty} |\tilde{\varphi}(k)|^2 dk. \quad (22)$$

This expression often represents a conservation principle. For instance, in quantum mechanics it is a conservation of probability [9]. In optics, it represents the fact that all the light passing through a diffraction aperture eventually appears distributed throughout the diffraction pattern [10]. On the other hand, since x and k represent arbitrary (canonical conjugate) variables, if φ were a function of time rather than space we would replace x by t and then k by the angular temporal frequency w to get

$$\varphi(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{\varphi}(w) e^{-iwt} dw, \quad \tilde{\varphi}(w) = \int_{-\infty}^{+\infty} \varphi(t) e^{iwt} dt \quad (23)$$

and

$$\int_{-\infty}^{+\infty} |\varphi(t)|^2 dt = \int_{-\infty}^{+\infty} |\tilde{\varphi}(w)|^2 dw. \quad (24)$$

Now, let us take a time depending wave $\varphi(t)$, defined at $x = 0$ by

$$\varphi(t) = \varphi_0 \Theta(t) e^{-\frac{\gamma}{2}t} \cos w_0 t, \quad \Theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases} \quad (25)$$

Function (25) is a transient oscillation as it has been defined in the above sections. From our experience with the previous cases we know that it is profitable to represent $\varphi(t)$ in terms of a complex function. In this case $\varphi = \text{Re}(Z)$, with

$$Z(t) = A(t)e^{-iw_0t}, \quad A(t) = \varphi_0\Theta(t)\exp\left(-\frac{\gamma}{2}t\right). \quad (26)$$

Observe that $|Z(t)|^2 = |A(t)|^2$. Then the Parseval formula (24) gives

$$\int_{-\infty}^{+\infty} |A(t)|^2 dt = \int_{-\infty}^{+\infty} |\tilde{A}(w)|^2 dw. \quad (27)$$

Since the stored energy at the time t is proportional to $|A(t)|^2$, both integrals in equation (27) give the total energy W of the wave as it is propagating throughout $x = 0$. Thereby the power involved in the oscillation as a function of time is given by $P(t) = dW/dt \propto |A(t)|^2$. In the same manner $I_w = dW/dw \propto |\tilde{A}(w)|^2$ is the energy per unit frequency interval. Now, from (26) we get $A(t) = Z(t)e^{iw_0t}$, so that

$$A(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{Z}(w)e^{-(w-w_0)t} dw \equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} a(\varepsilon)e^{-i\varepsilon t} d\varepsilon \quad (28)$$

where $\varepsilon := w - w_0$ and $a(\varepsilon) := \tilde{Z}(\varepsilon + w_0)$. This last term is given by

$$a(\varepsilon) = \int_{-\infty}^{+\infty} A(t)e^{i\varepsilon t} dt = \varphi_0 \int_0^{+\infty} e^{(i\varepsilon - \frac{\gamma}{2})t} dt = \frac{\varphi_0}{\frac{\gamma}{2} - i(w - w_0)}. \quad (29)$$

Then, up to a global constant, we have

$$I_w = \left(\frac{2\varphi_0}{\gamma}\right)^2 \frac{(\gamma/2)^2}{(w - w_0)^2 + (\gamma/2)^2}. \quad (30)$$

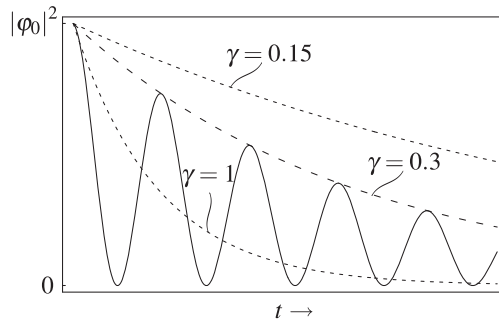


Figure 2: The power $P(t) \propto |\varphi_0|^2 e^{-\gamma t}$ involved with the transient oscillation (25) for the same values of γ as those given in Figure 1. Remark that the area under the dotted curves is larger for smaller values of the line breadth γ .

That is, the Fock-Breit-Wigner (FWB) function (30) is the spectral energy distribution of the transient oscillation (25). In the previous section we learned that the inverse of the damping constant γ measures the oscillation lifetime. The same rule holds for the

power $|A(t)|^2 = |\varphi_0|^2 e^{-\gamma t}$, as it is shown in Fig. 2. Let us investigate the extremal case of infinite lifetimes. Thus we calculate I_w in the limit $\gamma \rightarrow 0$. The result reads

$$I_w \rightarrow 2\pi \left(\frac{\varphi_0^2}{\gamma} \right) \delta(w - w_0), \quad \gamma \rightarrow 0 \quad (31)$$

where we have used

$$\delta(x) = \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \left(\frac{\epsilon}{x^2 + \epsilon^2} \right). \quad (32)$$

Infinite lifetimes ($1/\gamma = \tau \rightarrow +\infty$) correspond to spectral energy distributions of infinitesimal width ($\gamma \rightarrow 0$) and very high height (φ_0^2/γ). As a consequence, the transient oscillation (25) has a definite frequency ($w \rightarrow w_0$) along the time. The same conclusion is obtained for steady-state oscillations by taking $F_0^2 = 8m\varphi_0^2$ in equations (11–12). In the next sections we shall see that this lifetime \leftrightarrow width relationship links bound and decaying energy states in quantum mechanics.

As a very simple application of the above results let the plane wave (25) be the electric field emitted by an atom. Then W corresponds to the total energy radiated per unit area perpendicular to the direction of propagation. Equation (30) in turn, relates in quantitative way the behavior of the power radiated as a function of the time to the frequency spectrum of the energy radiated. To give a more involved example let us consider a nonrelativistic charged particle of mass m_e and charge q_e , acted on by an external force \vec{F} . The particle emits radiation since it is accelerated. To account for this radiative energy loss and its effect on the motion of the particle it is necessary to add a *radiative reaction force* \vec{F}_{rad} in the equation of motion to get

$$\vec{F} + \vec{F}_{\text{rad}} \equiv \vec{F} + \left(\frac{2q_e^2}{3c^3} \right) \frac{d^3}{dt^3} \vec{r} = m_e \frac{d^2}{dt^2} \vec{r} \quad (33)$$

with c the speed of light. This last expression is known as the *Abraham-Lorentz* equation and is useful only in the domain where the reactive term is a small correction, since the third order derivative term does not fulfill the requirements for a dynamical equation (see e.g., reference [11], Ch 16). Bearing this condition in mind let us investigate the effect of an external force of the form $\vec{F} = -m_e w_0^2 \vec{r}$. The Abraham-Lorentz equation is written

$$\left(\frac{2q_e^2}{3m_e c^3} \right) \frac{d^3}{dt^3} \vec{r} = \frac{d^2}{dt^2} \vec{r} + w_0^2 \vec{r}. \quad (34)$$

For small values of the third order term one has $\frac{d^2}{dt^2} \vec{r} \approx -w_0^2 \vec{r}$. That is, the particle oscillates like a mass at the end of a spring with frequency w_0 . Hence $\frac{d^3}{dt^3} \vec{r} \approx -w_0^2 \frac{d}{dt} \vec{r}$, so that the problem is reduced to the transient equation

$$\frac{d^2}{dt^2} \vec{r} + \gamma \frac{d}{dt} \vec{r} + w_0^2 \vec{r} = 0, \quad \gamma = \frac{2q_e^2 w_0^2}{3m_e c^3}, \quad (35)$$

the solution of which has the form (25-26) with $\varphi(t)$ replaced by $\vec{r}(t)$ and φ_0 by a constant vector \vec{r}_0 . To get an idea of the order of our approach let us evaluate the quotient γ/w_0^2 . A simple calculation gives the following constant

$$\frac{\gamma}{w_0^2} \approx 0.624 \times 10^{-23} \text{ s}. \quad (36)$$

Thus the condition $\gamma \ll 1s^{-1}$ defines the appropriate values of the frequency w_0 . For instance, let γ take the value $10^{-3}s^{-1}$. The appropriate value of w_0 is then of the order of an infrared frequency $w_0 \sim 10^{10}s^{-1}$. But if $\gamma \sim 10^{-11}s^{-1}$ then $w_0 \sim 10^6s^{-1}$, that is, the particle will oscillate at a radio wave frequency.

Under the limits of our approach the radiative reaction force \vec{F}_{rad} plays the role of a friction force which damps the oscillations of the electric field. The *resonant line shape* defined by the Fock-Breit-Wigner function (30) is broadened and shifted in frequency due to the reactive effects of radiation. That is, because the decaying of the power radiated $P(t) \propto |\varphi_0|^2 e^{-\gamma t}$, the emitted radiation corresponds to a pulse (wave train) with effective length $\lambda \approx c/\gamma$ and covering an interval of frequencies equal to γ rather than being monochromatic. The infinitesimal finiteness of the width in the spectral energy distribution (31) is then justified by the ‘radiation friction’. In the language of radiation the damping constant γ is known as the *line breadth*.

Finally, it is well known that the effects of radiative reaction are of great importance in the detailed behavior of atomic systems. It is then remarkable that the simple plausibility arguments discussed above led to the qualitative features derived from the formalism of quantum electrodynamics. By proceeding in a similar manner, it is also possible to verify that the scattering and absorption of radiation by an oscillator are also described in terms of FBW-like distributions appearing in the scattering cross section. The reader is invited to review the approach in classical references like [11, 12].

2.3 Fock’s Energy Distribution Model

Let $\{\phi_E(x)\}$ be a set of eigenfunctions belonging to energy eigenvalues E in the continuous spectrum of a given one-dimensional Hamiltonian H . The vectors are orthonormalized as follows

$$\int_{-\infty}^{\infty} \bar{\phi}_E(x) \phi_{E'}(x) dx = \delta(E' - E). \quad (37)$$

Notice we have taken for granted that the continuous spectrum is not degenerated, otherwise equation (37) requires some modifications. Let us assume that a wave function $\psi_0(x)$ can be expanded in a series of these functions, that is:

$$\psi_0(x) = \int_{-\infty}^{\infty} C(E) \phi_E(x) dE, \quad C(E) = \int_{-\infty}^{+\infty} \bar{\phi}_E(x) \psi_0(x) dx. \quad (38)$$

The inner product of ψ_0 with itself leads to the Parseval relation

$$W := (\psi_0, \psi_0) = \int_{-\infty}^{+\infty} |\psi_0(x)|^2 dx = \int_{-\infty}^{+\infty} |C(E)|^2 dE. \quad (39)$$

In the previous sections we learned that W allows the definition of the energy distribution $\omega(E)$. In this case we have

$$\omega(E) := \frac{dW}{dE} = |C(E)|^2. \quad (40)$$

At an arbitrary time $t > 0$ the state of the system reads

$$\psi_t(x) = \int_{-\infty}^{\infty} C(E) \phi_E(x) e^{-iEt/\hbar} dE. \quad (41)$$

The *transition amplitude* $T(t \geq 0)$ from the state ψ_0 into ψ_t is given by the inner product

$$T(t \geq 0) \equiv (\psi_0, \psi_t) = \int_{-\infty}^{+\infty} \bar{\psi}_0(x) \psi_t(x) dx = \int_{-\infty}^{+\infty} \omega(E) e^{-iEt/\hbar} dE. \quad (42)$$

Function T rules the transition probability $|T(t)|^2$ from $\psi_0(x)$ to $\psi_t(x)$ by relating the wave function at two different times: t_0 and $t \geq t_0$. It is known as the *propagator* in quantum mechanics and can be identified as a (spatial) Green's function for the time-dependent Schrödinger equation (see next section). From (42), it is clear that T can be investigated in terms of spatial coordinates x or as a function of the energy distribution. Next, following the Fock's arguments [9], we shall analyze the transition probability for a decaying system by assuming that $\omega(E)$ is given. Let $\omega(E)$ be the Fock-Breit-Wigner distribution

$$\omega(a) = \frac{1}{\pi} \left[\frac{(\Gamma/2)^2}{a^2 + (\Gamma/2)^2} \right] = \frac{1}{\pi} \left[\frac{(\Gamma/2)^2}{(a + i\Gamma/2)(a - i\Gamma/2)} \right], \quad a := E - E_0. \quad (43)$$

Then equation (42) reads

$$T(t \geq 0) = \frac{1}{\pi} \left(\frac{\Gamma}{2} \right)^2 e^{-iE_0 t/\hbar} \int_{-\infty}^{+\infty} \frac{e^{-iat/\hbar}}{(a + i\Gamma/2)(a - i\Gamma/2)} da. \quad (44)$$

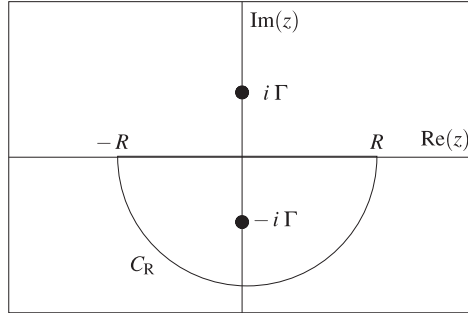


Figure 3: Contour of integration in the complex E -plane.

We start with the observation that function (43) has two isolated singularities at $a = \pm i\Gamma/2$ (none of them lies on the real axis!). When $R > 0$, the point $-i\Gamma/2$ lies in the interior of the semicircular region which is depicted in Fig. 3. At this stage, it is convenient to introduce the function

$$f(z) = \frac{g(z)}{z + i\Gamma/2}, \quad g(z) = \frac{e^{-izt/\hbar}}{z - i\Gamma/2}. \quad (45)$$

Integrating $f(z)$ counterclockwise around the boundary of the semicircular region the *Cauchy integral formula* (see e.g., [13]) is written

$$\int_R^{-R} f(a)da + \int_{C_R} f(z)dz = 2\pi ig(-i\Gamma/2). \quad (46)$$

This last expression is valid for all values of $R > 0$. Since the value of the integral on the right in (46) tends to 0 as $R \rightarrow +\infty$, we finally arrive at the desired result:

$$\int_{-\infty}^{+\infty} f(a)da = \frac{2\pi}{\Gamma} \exp\left(-\frac{\Gamma t}{2\hbar}\right). \quad (47)$$

In this way the transition rate $T(t)$ acquires the form of a transient oscillation

$$T(t \geq 0) = \frac{\Gamma}{2} \exp(-i\epsilon t/\hbar), \quad \epsilon := E_0 - i\Gamma/2. \quad (48)$$

It is common to find $T(t)$ as free of the factor $\Gamma/2$ (see e.g., [9], pp 159). This factor arises here because (43) has been written to be consistent with the previous expressions of a FWB distribution. The factor is easily removed if we take $\Gamma/2$ rather than $(\Gamma/2)^2$ in the numerator of $\omega(a)$. Now, we know that transient oscillations involve lifetimes and the present case is not an exception. Equation (48) means that the transition from $\psi_0(x)$ to $\psi_t(x)$ is an exponential decreasing function of the time. Since this rate of change is symmetrical, it also gives information about the rate of decaying of the initial wave. Thus, the probability that the system has not yet decayed at time t is given by

$$|T(t)|^2 = \left(\frac{\Gamma}{2}\right)^2 \exp(-\Gamma t/\hbar), \quad t \geq 0. \quad (49)$$

We note that the state of the undecayed system ψ_0 does not change but decays suddenly. That is, the time t in (49) is counted off starting from the latest instant when the system has not decayed. The above description was established by Fock in his famous book on quantum mechanics [9] and this is why functions like (43) bears his name. It is remarkable that the first Russian edition is dated on August 1931.

Finally, remark we have written (48) in terms of the complex number $\epsilon = E_0 - i\Gamma/2$. The reason is not merely aesthetic because, up to a constant factor, $T(t \geq 0)$ is the Fourier transform¹ of the expansion coefficient $C(E)$:

$$C(E) := \frac{\Gamma/2}{\sqrt{\pi}(E - E_0 + i\Gamma/2)} = \frac{\Gamma/2}{\sqrt{\pi}(E - \epsilon)} \quad (50)$$

where we have used (43). The relevance of this result will be clarified in the sequel.

¹The Fourier transform in this case corresponds to the equations (23), with the energy E and the angular frequency w related by the Einstein's expression $E = \hbar w$.

3 Quanta, Tunneling and Resonances

Let us consider the motion of a particle of mass m constrained to move on the straight-line in a given potential $U(x)$. Its *time-dependent Schrödinger equation* is

$$H\psi(x, t) := \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t). \quad (51)$$

Let us assume the wave-function $\psi(x, t)$ is separable, that is $\psi(x, t) = \varphi(x)\theta(t)$. A simple calculation leads to $\theta(t) = \exp(-iEt/\hbar)$, with E a constant, and $\varphi(x)$ a function fulfilling

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right] \varphi(x) \equiv H\varphi(x) = E\varphi(x). \quad (52)$$

This time-independent Schrödinger equation (plainly the Schrödinger equation) defines a set of *eigenvalues* E and *eigenfunctions* of the Hamiltonian operator H which, in turn, represents the *observable* of the energy. Now, to get some intuition about the separableness of the wave-function let us take the Fourier transform of its temporal term

$$\tilde{\theta}(E) = \lim_{a \rightarrow +\infty} \int_{-a}^a e^{i(E-E')t/\hbar} dt = 2\pi\delta(E - E') \quad (53)$$

where we have used (18). This last result means that the energy distribution is of infinitesimal width and very high height. In other words, the system has a definite energy $E = E'$ along the time. Systems exhibiting this kind of behavior are known as *stationary* and it is said that they are *conservative*. Since the Hamiltonian operator H does not depend on t and because for any analytic function f of H one has

$$f(H)\varphi(x) = f(E)\varphi(x) \quad (54)$$

our separability ansatz $\psi \rightarrow \varphi\theta$ can be written

$$\psi(x, t) = \exp\left(-\frac{i}{\hbar}Ht\right) \varphi(x) = e^{-iEt/\hbar} \varphi(x). \quad (55)$$

According with the Born's interpretation, the wave function $\varphi(x)$ defines the probability density $\rho(x) = |\varphi(x)|^2$ of finding the quantum particle between x and $x + dx$. Thereby, the sum of all probabilities (i.e., the probability of finding the particle anywhere in the straight-line at all) is unity:

$$\int_{-\infty}^{+\infty} \rho(x) dx = \int_{-\infty}^{+\infty} \overline{\varphi}(x) \varphi(x) dx \equiv \int_{-\infty}^{+\infty} |\varphi(x)|^2 dx = 1. \quad (56)$$

The above equation represents the *normalization condition* fulfilled by the solutions $\varphi(x)$ to be physically acceptable. Hence, they are elements of a vector space \mathcal{H} consisting of *square-integrable* functions and denoted as $\mathcal{H} = L^2(\mathbf{R}, \mu)$, with μ the Lebesgue measure (for simplicity in notation we shall omit μ by writing $L^2(\mathbf{R})$). As an example, \mathcal{H} can be the

space spanned by the Hermite polynomials $H_n(x)$, weighted by the factor $\mu(x) = e^{-x^2/2}$ and defined as follows

$$H_n(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} e^{-x^2/2}. \quad (57)$$

In quantum mechanics, observables are represented by the so-called Hermitian operators in the Hilbert space \mathcal{H} . A differential operator A defined on $L^2(\mathbf{R})$ is said to be *Hermitian* if, whenever Af and Ag are defined for $f, g \in L^2(\mathbf{R})$ and belong to $L^2(\mathbf{R})$, then

$$(Af, g) = (f, Ag) = \int_{-\infty}^{+\infty} \overline{f}(x) Ag(x) \mu(x) dx. \quad (58)$$

In particular, if $f = g$ the above definition means that the action of the Hermitian operator A on $f \in L^2(\mathbf{R})$ is symmetrical. If $Af(x) = \alpha f(x)$, we have $(Af, f) = \overline{\alpha}$ and $(f, Af) = \alpha$, so that $\overline{\alpha} = \alpha \Rightarrow \alpha \in \mathbf{R}$. In other words, the eigenvalues of a Hermitian operator acting on $L^2(\mathbf{R})$ are real numbers. It is important to stress, however, that this rule is not true in the opposite direction. In general, as we are going to see in the next sections, there is a wide family of operators A_λ sharing the same set of real eigenvalues $\{\alpha\}$. (The family includes some non-Hermitian operators!) Moreover, notice that the rule is not necessarily true if $f(x) \notin L^2(\mathbf{R})$. In general, the set of solutions of $Af(x) = \alpha f(x)$ is wider than $L^2(\mathbf{R})$. That is, the complete set of mathematical solutions $\varphi(x)$ embraces functions such that its absolute value $|\varphi(x)|$ diverges even for real eigenvalues. A plain example is given by the solutions representing scattering states because they do not fulfill (56). In such a case one introduces another kind of normalization like that defined in (37), with a similar notion of the Born's probability as we have seen in the previous section. Normalization (56) is then a very restrictive condition picking out the appropriate physical solutions among the mathematical ones. This is why the Schrödinger equation (51) is “physically solvable” for a very narrow set of potentials.

If E is real, the time-dependent factor in (55) is purely oscillatory (a phase) and the time displacement $\psi(x, t)$ gives the same ‘prediction’ (probability density) as $\varphi(x)$. As a result, both of these vectors lead to the same expectation values of the involved observables

$$\langle A \rangle := \int_{-\infty}^{+\infty} \overline{\psi}(x, t) A \psi(x, t) dx = \int_{-\infty}^{+\infty} \overline{\varphi}(x) A \varphi(x) = \alpha. \quad (59)$$

In particular, $\langle H \rangle = E$ shows that the eigenvalue E is also the expectation value of the energy. Notice that stationary states are states of well-defined energy, E being the definite value of its energy and not only its expectation value (see equation 53). That is, any determination of the energy of the particle always yields the particular value E . Again, as an example, let us consider a scattering state. Far away from the influence of the scatterer, it is represented by a plane wave like

$$\psi(x, t) = \exp\left(-\frac{i}{\hbar} Et\right) \exp\left(-\frac{i}{\hbar} xp\right) \quad (60)$$

where p is the linear momentum of the particle. Function (60) represents a state having a definite value for its energy. However, there is no certainty neither on the position of the particle nor in the transit time of the particle at a given position. In general, the energy

distribution will not be a continuous function. It could include a set of isolated points (discrete energy levels) and/or continuous portions showing a set of very narrow and high peaks (resonance levels). The former correspond to infinite lifetime states (the observed discrete energy levels of atoms are good examples) while the lifetime of the second ones will depend on the involved interactions.

3.1 Quasi-stationary States and Optical Potentials

It is also possible to define a *probability current density* j

$$j = \frac{\hbar}{2mi} \left[\bar{\psi} \left(\frac{d}{dx} \psi \right) - \left(\frac{d}{dx} \bar{\psi} \right) \psi \right] \quad (61)$$

which, together with the probability density $\rho = |\psi|^2$ satisfies a continuity equation

$$\frac{d\rho}{dt} + \frac{dj}{dx} = 0 \quad (62)$$

exactly as in the case of conservation of charge in electrodynamics. Observe that stationary states fulfill $d\rho/dt = 0$, so that $\rho \neq \rho(t)$ and $j = 0$. What about decaying systems for which the transition amplitude $T(t \geq 0)$ involves a complex number $\epsilon = E_0 - i\Gamma/2$ like that found in equation (48)? Let us assume a complex eigenvalue of the energy $H\varphi_\epsilon = \epsilon\varphi_\epsilon$ is admissible in (55). Then we have $\rho(x, t) = \rho_\epsilon(x)e^{-\Gamma t/\hbar}$ and $j \neq 0$. That is, complex energies are included at the cost of adding a non-trivial value of the probability current density j . A conventional way to solve this ‘problem’ is to consider a complex potential $U = U_R + iU_I$. Then equation (62) acquires the form

$$\frac{d\rho}{dt} + \frac{dj}{dx} = \frac{2}{\hbar} U_I(x) \rho(x), \quad (63)$$

the integration of which can be identified with the variation of the number of particles

$$\frac{d}{dt} N = \frac{2}{\hbar} \int_{-\infty}^{+\infty} U_I(x) \rho(x) dx. \quad (64)$$

Let $U_I(x) = U_0$ be a constant. If $U_0 > 0$, there is an increment of the number of particles ($dN/dt > 0$) and viceversa, $U_0 < 0$ leads to a decreasing number of particles ($dN/dt < 0$). In the former case the imaginary part of the potential works like a source of particles while the second one shows U_I as a sink of particles. The introduction of this potential into the Schrödinger equation gives

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U_R(x) + iU_0 \right] \varphi_\epsilon(x) = \left(E_0 - i\frac{\Gamma}{2} \right) \varphi_\epsilon(x). \quad (65)$$

Then, the identification $U_0 = -\Gamma/2$ reduces the solving of this last equation to a stationary problem. The exponential decreasing probability density $\rho_\epsilon(x)e^{-\Gamma t/\hbar}$ is then justified by the presence of a sink-like potential $U_I(x) = U_0 < 0$. However, this solution requires the introduction of a non-Hermitian Hamiltonian because the involved potential is complex.

Although such a Hamiltonian is not an observable in the sense defined in the above section, notice that $U_0 = -i\Gamma/2$ is a kind of damping constant. The lifetime of the probability $\rho(x, t)$ is defined by the inverse of Γ and, according with the derivations of the previous section, the energy distribution shows a bell-shaped peak at $E = E_0$. In other words, the complex eigenvalue $\epsilon = E_0 - i\Gamma/2$ is a pole of $\omega(E)$ and represents a resonance of the system. The modeling of decay by the use of complex potentials with constant imaginary part is known as the *optical model* in nuclear physics. The reason for such a name is clarified in the next section.

3.1.1 Complex Refractive index in Optics

It is well known that the spectrum of *electromagnetic energy* includes radio waves, infrared radiation, the visible spectrum of colors red through violet, ultraviolet radiation, x -rays and gamma radiation. All of them are different forms of light and are usually described as *electromagnetic waves*. The physical theory treating the *propagation* of light is due mainly to the work of James Clerk Maxwell (1831-1879). The interaction of light and matter or the absorption and emission of light, on the other hand, is described by the quantum theory. Hence, a consistent theoretical explanation of all optical phenomena is furnished jointly by Maxwell's electromagnetic theory and the quantum theory. In particular, the speed of light $c = 299,792,456.2 \pm 1.1 \text{ m/s}$ is a part of the *wave equation* fulfilled by the electric field \vec{E} and the magnetic field \vec{H} :

$$\nabla^2 \vec{A} = \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2}, \quad \vec{A} = \vec{E}, \vec{H}. \quad (66)$$

The above expression arises from the Maxwell's equations in empty space with $c = (\mu_0 \epsilon_0^*)^{-1/2}$. The constant μ_0 is known as the *permeability of the vacuum* and the constant ϵ_0^* is called the *permittivity of the vacuum* [11]. In isotropic nonconducting media these constants are replaced by the corresponding constants for the medium, namely μ and ϵ^* . Consequently, the speed of propagation ν of the electromagnetic fields in a medium is given by $\nu = (\mu \epsilon^*)^{-1/2}$. The *index of refraction* n is defined as the ratio of the speed of light in vacuum to its speed in the medium: $n = c/\nu$. Most transparent optical media are nonmagnetic so that $\mu/\mu_0 = 1$, in which case the index of refraction should be equal to the square root of the relative permittivity $n = (\epsilon^*/\epsilon_0^*)^{1/2} \equiv K^{1/2}$. In a nonconducting, isotropic medium, the electrons are permanently bound to the atoms comprising the medium and there is no preferential direction. This is what is meant by a simple isotropic dielectric such as glass [14]. Now, consider a (one-dimensional) plane harmonic wave incident upon a plane boundary separating two different optical media. In agreement with the phenomena of reflection and refraction of light ruled by the Huygen's principle, there will be a reflected wave and a transmitted wave (see e.g. [10]). Let the first medium be the empty space and the second one having a complex index of refraction

$$\mathcal{N} = n + in_I. \quad (67)$$

Then, the wavenumber of the refracted wave is complex:

$$\mathcal{K} = k + i\alpha \quad (68)$$

and we have

$$\begin{aligned}\vec{E} &= \vec{E}_0 e^{i(k_0 x - wt)} && \text{(incident wave)} \\ \vec{E}' &= \vec{E}'_0 e^{i(k'_0 x - wt)} && \text{(reflected wave)} \\ \vec{E}'' &= \vec{E}''_0 e^{i(\mathcal{K}x - wt)} = \vec{E}''_0 e^{-\alpha x} e^{i(kx - wt)} && \text{(refracted wave)}\end{aligned}$$

If $\alpha > 0$ the factor $e^{-\alpha x}$ indicates that the amplitude of the wave decreases exponentially with the distance. That is, the energy of the wave is absorbed by the medium and varies with distance as $e^{-2\alpha x}$. Hence 2α is the *coefficient of absorption* of the medium. The imaginary part n_I of \mathcal{N} , in turn, is known as the *extinction index*. In general, it can be shown that the corresponding polarization is similar to the amplitude formula for a driven harmonic oscillator [14]. Thus, an optical resonance phenomenon will occur for light frequencies in the neighborhood of the resonance frequency $w_0 = (K/m)^{1/2}$. The relevant aspect of these results is that a complex index of refraction \mathcal{N} leads to a complex wavenumber \mathcal{K} . That is, the properties of the medium (in this case an absorbing medium) induce an specific behavior of the electromagnetic waves (in this case, the exponentially decreasing of the amplitude). This is the reason why the complex potential discussed in the previous section is named the ‘optical potential’.

3.2 Quantum Tunneling and Resonances

In quantum mechanics the complex energies were studied for the first time in a paper by Gamow concerning the alpha decay (1928) [1]. In a simple picture, a given nucleus is composed in part by alpha particles (${}^4_2\text{He}$ nuclei) which interact with the rest of the nucleus via an attractive well (obeying the presence of nuclear forces) plus a potential barrier (due, in part, to repulsive electrostatic forces). The former interaction constrains the particles to be bounded while the second holds them inside the nucleus. The alpha particles have a small (non-zero) probability of tunneling to the other side of the barrier instead of remaining confined to the interior of the well. Outside the potential region, they have a finite lifetime. Thus, alpha particles in a nucleus should be represented by *quasi-stationary* states. For such states, if at time $t = 0$ the probability of finding the particle inside the well is unity, in subsequent moments the probability will be a slowly decreasing function of time (see e.g. Sections 7 and 8 of reference [9]). In his paper of 1928, Gamow studied the escape of alpha particles from the nucleus via the tunnel effect. In order to describe eigenfunctions with exponentially decaying time evolution, Gamow introduced energy eigenfunctions ψ_G belonging to complex eigenvalues $Z_G = E_G - i\Gamma_G$, $\Gamma_G > 0$. The real part of the eigenvalue was identified with the energy of the system and the imaginary part was associated with the inverse of the lifetime. Such ‘decaying states’ were the first application of quantum theory to nuclear physics.

Three years later, in 1931, Fock showed that the law of decay of a quasi-stationary state depends only on the energy distribution function $\omega(E)$ which, in turn, is meromorphic [9]. According to Fock, the analytical expression of $\omega(E)$ is rather simple and has only two poles $E = E_0 \pm i\Gamma$, $\Gamma > 0$ (see our equation (43) and equation (8.13) of [9]). A close result was derived by Breit and Wigner in 1936. They studied the cross section of

slow neutrons and found that the related energy distribution reaches its maximum at E_R with a half-maximum width Γ_R . A resonance is supposed to take place at E_R and to have “half-value breath” Γ_R [2]. It was in 1939 that Siegert introduced the concept of a purely outgoing wave belonging to the complex eigenvalue $\epsilon = E - i\Gamma/2$ as an appropriate tool in the studying of resonances [15]. This complex eigenvalue also corresponds to a first-order pole of the S matrix [16] (for more details see e.g. [17]). However, as the Hamiltonian is a Hermitian operator, then (in the Hilbert space \mathcal{H}) there can be no eigenstate having a strict complex exponential dependence on time. In other words, decaying states are an approximation within the conventional quantum mechanics framework. This fact is usually taken to motivate the study of the rigged (equipped) Hilbert space $\overline{\mathcal{H}}$ [3–5] (For a recent review see [6]). The mathematical structure of $\overline{\mathcal{H}}$ lies on the nuclear spectral theorem introduced by Dirac in a heuristic form [18] and studied in formal rigor by Maurin [19] and Gelfand and Vilenkin [20].

In general, solutions of the Schrödinger equation associated to complex eigenvalues and fulfilling purely outgoing conditions are known as *Gamow-Siegert functions*. If u is a function solving $Hu = \epsilon u$, the appropriate boundary condition may be written

$$\lim_{x \rightarrow \pm\infty} (u' \mp iku) = \lim_{x \rightarrow \pm\infty} \{(-\beta \mp ik) u\} = 0, \quad (69)$$

with β defined as the derivative of the logarithm of u :

$$\beta := -\frac{d}{dx} \ln u. \quad (70)$$

Now, let us consider a one-dimensional short-range potential $U(x)$, characterized by a cutoff parameter $\zeta > 0$. The general solution of (52) can be written in terms of ingoing and outgoing waves:

$$u_{<} := u(x < -\zeta) = Ie^{ikx} + Le^{-ikx}, \quad u_{>} := u(x > \zeta) = Ne^{-ikx} + Se^{ikx} \quad (71)$$

where the coefficients I, L, N, S , depend on the potential parameters and the incoming energy $k^2 = 2m\epsilon/\hbar^2$ (the kinetic parameter k is in general a complex number $k = k_R + ik_I$), they are usually fixed by imposing the continuity conditions for u and du/dx at the points $x = \pm\zeta$. Among these solutions, we are interested in those which are purely outgoing waves. Thus, the second term in each of the functions (71) must dominate over the first one. For such states, equation (61) takes the form:

$$j_{<} = -v|u_{<}|^2, \quad j_{>} = v|u_{>}|^2, \quad v := \frac{\hbar}{2m}(k + \bar{k}) = \frac{\hbar k_R}{m}. \quad (72)$$

This last equation introduces the *flux velocity* v . If ϵ is a real number $\epsilon = E$, then k is either pure imaginary or real according to E negative or positive. If we assume that the potential admits negative energies, we get $k_{\pm} = \pm i\sqrt{|2mE/\hbar^2|}$ and (72) vanishes (the flux velocity $v \propto k_R$ is zero outside the interaction zone). Notice that the solutions $u_E^{(+)}$, connected with k_+ , are bounded so that they are in $L^2(\mathbf{R})$. That is, they are the physical solutions φ associated with a discrete set of eigenvalues $2mE_n/\hbar^2 = k_{n,+}^2$ solving the continuity equations for u and du/dx at $x = \pm\zeta$. On the other hand, *antibound states*

$u_E^{(-)}$ increase exponentially as $|x| \rightarrow +\infty$. To exhaust the cases of a real eigenvalue ϵ , let us take now $2mE/\hbar^2 = \kappa^2 > 0$. The outgoing condition (69) drops the interference term in the density

$$\rho(x; t) = |N|^2 + |S|^2 + 2|\overline{N}S| \cos(2\kappa x + \text{Arg } S/N), \quad x > \zeta, \quad (73)$$

so that the integral of $\rho = |S|^2$ is not finite neither in space nor in time (similar expressions hold for $x < -\zeta$). Remark that flux velocity is not zero outside the interaction zone. Thereby, $E > 0$ provides outgoing waves at the cost of a net outflow $j \neq 0$. To get solutions which are more appropriate for this nontrivial j , we shall consider complex eigenvalues ϵ . Let us write

$$\epsilon = E - \frac{i}{2}\Gamma, \quad \epsilon_R \propto k_R^2 - k_I^2, \quad \epsilon_I \propto 2k_R k_I \quad (74)$$

where $2m\epsilon/\hbar^2 = (k_R + ik_I)^2$. According to (69), the boundary condition for β reads now

$$\lim_{x \rightarrow \pm\infty} \{-\beta \pm (k_I - ik_R)\} = 0 \quad (75)$$

so that the flux velocity is $v_+ \propto k_R$ for $x > \zeta$ and $v_- \propto -k_R$ for $x < -\zeta$. Hence, the “correct” direction in which the outgoing waves move is given by $k_R > 0$. In this case, the density

$$\rho(x; t) \equiv |u(x, t)|^2 = e^{-\Gamma t/\hbar} |u(x)|^2, \quad \lim_{x \rightarrow \pm\infty} \rho(x; t) \propto e^{-\Gamma(t-x/v_{\pm})/\hbar} \quad (76)$$

can be damped by taking $\Gamma > 0$. Thereby, $k_I \neq 0$ and $k_R \neq 0$ have opposite signs. Since $k_R > 0$ has been previously fixed, we have $k_I < 0$. Then, purely outgoing, exponentially increasing functions (resonant states) are defined by points in the fourth quadrant of the complex k -plane. In general, it can be shown that the *transmission amplitude* S in (71) is a meromorphic function of k , with poles restricted to the positive imaginary axis (bound states) and the lower half-plane (resonances) [21]. Let k_n be a pole of S in the fourth quadrant of the k -plane, then $-\overline{k}_n$ is also a pole while \overline{k}_n and $-k_n$ are zeros of S (see Figure 4, left). On the other hand, if S is studied as a function of ϵ , a Riemann surface of $\epsilon^{1/2} = k$ is obtained by replacing the ϵ -plane with a surface made up of two sheets R_0 and R_1 , each cut along the positive real axis and with R_1 placed in front of R_0 (see e.g. [13], pp 337). As the point ϵ starts from the upper edge of the slit in R_0 and describes a continuous circuit around the origin in the counterclockwise direction (Figure 4, right), the angle increases from 0 to 2π . The point then passes from the sheet R_0 to the sheet R_1 , where the angle increases from 2π to 4π . The point then passes back to the sheet R_0 and so on. Complex poles of $S(\epsilon)$ always arise in conjugate pairs (corresponding to k and $-\overline{k}$) while poles on the negative real axis correspond to either bound or antibound states.

Observe that density (76) increases exponentially for either large $|x|$ or large negative values of t . The usual interpretation is that the compound (φ_ϵ, V) represents a decaying system which emitted waves in the remote past $t - x/v$. As it is well known, the long lifetime limit ($\Gamma \rightarrow 0$) is useful to avoid some of the complications connected with the limit $t \rightarrow -\infty$ (see discussions on time asymmetry in [22]). In this context, one usually imposes the condition:

$$\frac{\Gamma/2}{\Delta E} < 1. \quad (77)$$

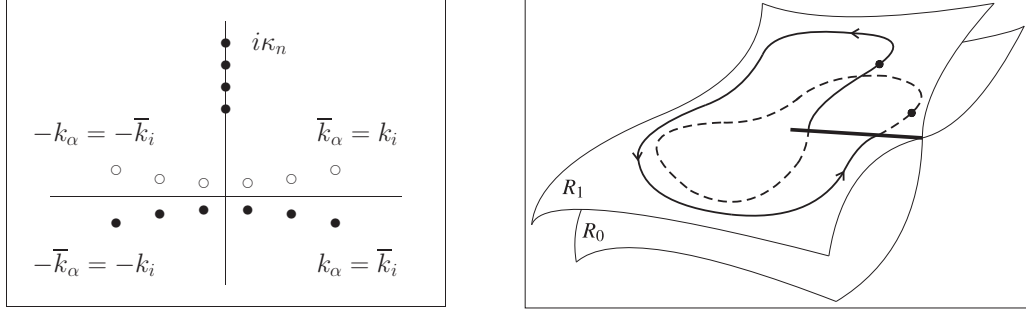


Figure 4: **Left:** Schematic representation of the poles (disks) and the zeros (circles) of the transmission amplitude $S(k)$ in the complex k -plane. Bounded energies correspond to poles located on the positive imaginary axis **Right:** The two-sheet Riemann surface $\sqrt{\epsilon} = k$. The lower edge of the slit in R_0 is joined to the upper edge of the slit in R_1 , and the lower edge of the slit in R_1 is joined to the upper edge of the slit in R_0 . The picture is based on the description given by J.M. Brown and R.V. Churchill in ref. [13].

Thus, the level width Γ must be much smaller than the level spacing ΔE in such a way that closer resonances imply narrower widths (longer lifetimes). In general, the main difficulty is precisely to find the adequate E and Γ . However, for one-dimensional stationary short range potentials, in [21] it has been shown that the superposition of a denumerable set of FBW distributions (each one centered at each resonance $E_n, n = 1, 2, \dots$) entails an approximation of the coefficient T such that the larger the number N of close resonances involved, the higher the precision of the approximation (see Fig. 5):

$$T \approx \omega_N(\epsilon_R) = \sum_{n=1}^N \omega(\epsilon_R, E_n) \quad (78)$$

with

$$\omega(\epsilon_R, E) = \frac{(\Gamma/2)^2}{(\epsilon_R - E)^2 + (\Gamma/2)^2}. \quad (79)$$

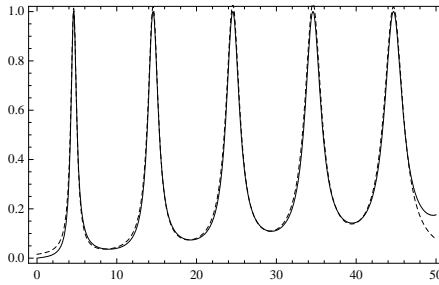


Figure 5: Functions T and ω_N (dotted curve) for a square well with strength $V_0 = 992.25$ and weigh $b = 20$ for which the FBW sum matches well the transmission coefficient for the first five resonances [23] (see also [21]).

Processes in which the incident wave falls upon a single scatterer are fundamental in the study of more involved interactions [24]. In general, for a single target the scattering amplitude is a function of two variables (e.g. energy and angular momentum). The above model corresponds to the situation in which one of the variables is held fixed (namely, the

angular momentum). A more realistic three dimensional model is easily obtained from these results: even functions are dropped while an infinitely extended, impenetrable wall is added at the negative part of the straight line [25]. Such a situation corresponds to s -waves interacting with a single, spherically symmetric, square scatterer (see e.g. [26]).

3.3 Complex Scaling Method

Some other approaches extend the framework of quantum theory so that quasi-stationary states can be defined in a precise form. For example, the complex-scaling method [7, 8, 27] (see also [28]) embraces the transformation $H \rightarrow UHU^{-1} = H_\theta$, where U is the complex-scaling operator $U = e^{-\theta XP/\hbar}$, with θ a dimensionless parameter and $[X, P] = i\hbar$. The transformation is achievable by using the Baker-Campbell-Hausdorff formulae [29]:

$$e^A B e^{-A} = \{e^A, B\} = \sum_{n=0}^{\infty} \frac{1}{n!} \{A^n, B\} \quad (80)$$

with A and B two arbitrary linear operators and

$$\{A^n, B\} = \underbrace{[A, [A, \dots [A, B] \dots]]}_{n \text{ times}}.$$

The identification $A = -\theta XP/\hbar$ and $B = X$ leads to

$$UXU^{-1} = \sum_{n=0}^{\infty} \frac{1}{n!} (i\theta)^n X = e^{i\theta} X, \quad UPU^{-1} = \sum_{n=0}^{\infty} \frac{1}{n!} (-i\theta)^n P = e^{-i\theta} P, \quad (81)$$

where we have used

$$\{(XP)^n, X\} = (-i\hbar)^n X, \quad \{(XP)^n, P\} = (i\hbar)^n P. \quad (82)$$

The following calculations are now easy

$$\begin{aligned} UP^2U^{-1} &= (UPU^{-1})(UPU^{-1}) = (UPU^{-1})^2 = e^{-2i\theta} P^2, \\ UV(X)U^{-1} &= U \left(\sum_{k=0}^{\infty} \frac{1}{k!} V_k X^k \right) U^{-1} = V(e^{i\theta} X). \end{aligned} \quad (83)$$

So that we finally get

$$UHU^{-1} \equiv H_\theta = e^{-2i\theta} P^2 + V(e^{i\theta} X). \quad (84)$$

Remark that in the Schrödinger's representation we have

$$X = x, \quad P = -i\hbar \frac{d}{dx}, \quad U = e^{i\theta x d/dx} \Rightarrow Uf(x) = f(xe^{i\theta}). \quad (85)$$

This transformation converts the description of resonances by non-integrable Gamow-Siegert functions into one by square integrable functions. Let $k = |k|e^{i\alpha} \equiv |k|e^{-i\beta}$ be

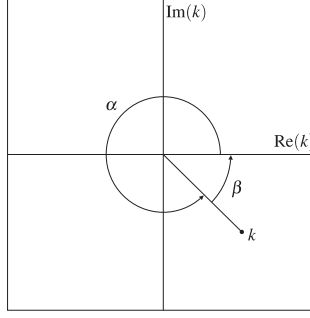


Figure 6: Polar form of an arbitrary point on the complex k -plane.

a point on the complex k -plane (see Figure 6). If k lies on the fourth quadrant then $0 < \beta < \pi/2$ and the related Gamow-Siegert function u_ϵ behaves as follows

$$u_\epsilon(x \rightarrow \pm\infty) \sim e^{\pm i|k|x \cos \beta} e^{\pm |k|x \sin \beta}. \quad (86)$$

That is, u_ϵ diverges for large values of $|x|$. The behavior of the complex-scaled function $\tilde{u}_\epsilon = U(u_\epsilon)$, on the other hand, reads

$$\tilde{u}_\epsilon(x \rightarrow \pm\infty) \sim e^{\pm i|k|x \cos(\theta-\beta)} e^{\mp |k|x \sin(\theta-\beta)}. \quad (87)$$

Thereby, \tilde{u}_ϵ is a bounded function if $\theta - \beta > 0$, i.e., if $\tan \theta > \tan \beta$. The direct calculation shows that complex-scaling preserves the square-integrability of the bounded states φ_n , whenever $0 < \theta < \pi/2$. Then one obtains

$$0 < \theta - \beta < \pi/2. \quad (88)$$

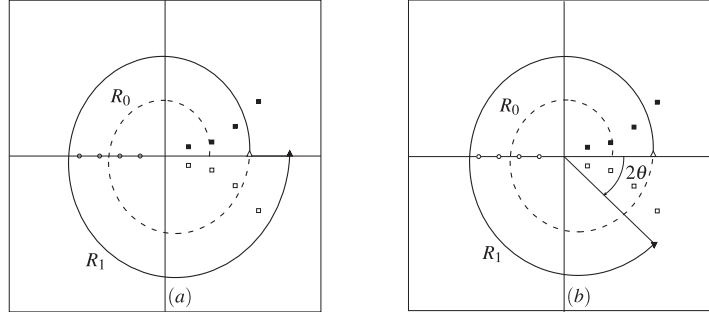


Figure 7: **Left.** Schematic representation of the two-sheet Riemann surface showed in Figure 4. Dashed curves and empty squares lie on the first sheet R_0 , continuous curves and filled squares lie on the second sheet R_1 **Right.** The complex rotated plane ‘exposing’ the resonant poles lying on the first sheet R_0 .

As regards the complex-scaled scattering states we have

$$e^{\pm i|k|x} \rightarrow e^{\pm i|k|x \cos \theta} e^{\mp |k|x \sin \theta}. \quad (89)$$

So that plane waves are transformed into exponential decreasing or increasing functions for large values of $|x|$. To preserve the oscillating form of scattering wave-functions the kinetic

parameter k has to be modified. That is, the transformation $k = |k| \rightarrow |k|e^{-i\theta}$ reduces (89) to the conventional plane-wave form of the scattering states. This transformation, however, induces a rotation of the positive real axis in the clockwise direction by the angle 2θ : $E \propto k^2 \rightarrow |k|^2 e^{-i2\theta} \propto E e^{-i2\theta}$. That is, the rotated energy is complex $\epsilon = E_R - i\Gamma/2$ with $E_R = E \cos(2\theta)$, $\Gamma/2 = \sin(2\theta)$. In summary, complex rotation is such that: 1) Bound state poles remain unchanged under the transformation 2) Cuts are now rotated downward making an angle of 2θ with the real axis 3) Resonant poles are ‘exposed’ by the cuts (see Figure 7). Another relevant aspect of the method is that it is possible to construct a resolution to the identity [30]. Moreover, as the complex eigenvalues are θ -independent, the resonance phenomenon is just associated with the discrete part of the complex-scaled Hamiltonian [31] (but see [28]). As a final remark, let us emphasize that complex-scaling ‘regularizes’ the divergent Gamow-Siegert functions u_ϵ at the cost of introducing a non-Hermitian Hamiltonian H_θ . From equation (84) we get

$$H_\theta^\dagger = e^{i2\theta} P^2 + V(e^{-i\theta} R) \neq H_\theta. \quad (90)$$

In other words, the ‘regularized’ solutions \tilde{u}_ϵ are square-integrable eigenfunctions of a complex potential $V(e^{i\theta} x)$ belonging to the complex eigenvalue ϵ .

3.4 Darboux-Gamow Transformations

In a different survey, complex eigenvalues of Hermitian Hamiltonians have been used to implement Darboux (supersymmetric) transformations in quantum mechanics [32–37] (see also the discussion on ‘atypical models’ in [38]). The transformed Hamiltonians include non-Hermitian ones, for which the point spectrum sometimes has a single complex eigenvalue [21, 25, 33–35]. This last result, combined with appropriate squeezing operators [39], could be in connection with the complex-scaling technique. In general, supersymmetric transformations constitute a powerful tool in quantum mechanics [38]. However, as far as we know, until the recent results reported in [21, 25, 35, 36] the connection between supersymmetric transformations and resonant states has been missing. In this context and to throw further light on the complex function β we may note that (70) transforms the Schrödinger equation (52) into a Riccati one

$$-\beta' + \beta^2 + \epsilon = V \quad (91)$$

where we have omitted the units. Remark that (91) is not invariant under a change in the sign of the function β :

$$\beta' + \beta^2 + \epsilon = V + 2\beta'. \quad (92)$$

These last equations define a Darboux transformation $\tilde{V} \equiv \tilde{V}(x, \epsilon) = V(x) + 2\beta'(x)$ of the initial potential V . This transformation necessarily produces a complex function if u in equation (70) is a Gamow-Siegert function u_ϵ . That is, a *Darboux-Gamow deformation* is defined as follows [21]:

$$\tilde{V} = V + 2\beta' \equiv V - 2 \frac{d^2}{dx^2} \ln u_\epsilon. \quad (93)$$

The main point here is that the purely outgoing condition (69) leads to $\beta' \rightarrow 0$ so that $\tilde{V} \rightarrow V$, in the limit $|x| \rightarrow +\infty$. In general, according with the excitation level of the transformation function u_ϵ , the real \tilde{V}_R and imaginary \tilde{V}_I parts of \tilde{V} show a series of maxima and minima. Thus, the new potential behaves as an optical device emitting and absorbing probability flux at the same time, since the function $I_I(x)$ shows multiple changes of sign [21, 25, 35, 36]. On the other hand, the solutions $y \equiv y(x, \epsilon, \mathcal{E})$ of the non-Hermitian Schrödinger equation

$$-y'' + \tilde{V}y = \mathcal{E}y \quad (94)$$

are easily obtained

$$y \propto \frac{W(u_\epsilon, \psi)}{u_\epsilon}, \quad (95)$$

where $W(*, *)$ stands for the Wronskian of the involved functions and ψ is eigen-solution of (94) with eigenvalue \mathcal{E} . It is easy to show that scattering waves and their Darboux-Gamow deformations share similar transmission probabilities [21]. Now, let us suppose that Hamiltonian H includes a point spectrum $\sigma_d(H) \subset \text{Sp}(H)$. If ψ_n is a (square-integrable) eigenfunction with eigenvalue \mathcal{E}_n , then its Darboux-Gamow deformation (95) is bounded:

$$\lim_{x \rightarrow \pm\infty} y_n = \mp(\sqrt{\mathcal{E}_n} + ik)(\lim_{x \rightarrow \pm\infty} \psi_n). \quad (96)$$

Thereby, y_n is a normalizable eigenfunction of \tilde{H} with eigenvalue \mathcal{E}_n . However, as ϵ is complex, although the new functions $\{y_n\}$ may be normalizable, they will not form an orthogonal set [34] (see also [40] and the ‘puzzles’ with self orthogonal states [41]). There is still another bounded solution to be considered. Function $y_\epsilon \propto \varphi_\epsilon^{-1}$ fulfills equation (94) for the complex eigenvalue ϵ . Since $\lim_{x \rightarrow \pm\infty} |y_\epsilon|^2 = e^{\pm 2k_I x}$ and $k_I < 0$, we have another normalizable function to be added to the set $\{y_n\}$.

In summary, one is able to construct non-Hermitian Hamiltonians \tilde{H} for which the point spectrum is also $\sigma_d(H)$, extended by a single complex eigenvalue $\text{Sp}(\tilde{H}) = \text{Sp}(H) \cup \{\epsilon\}$. As we can see, the results of the Darboux-Gamow deformations are quite similar to those obtained by means of the complex-scaling method. This relationship deserves a detailed discussion which will be given elsewhere.

4 Conclusions

We have studied the concept of *resonance* as it is understood in classical mechanics by analyzing the motion of a forced oscillator with damping. The resonance phenomenon occurs for steady state oscillations when the driving force oscillates at an angular frequency equal to the natural frequency w_0 of the oscillator. Then the amplitude of the oscillation is maximum and w_0 is called the resonance frequency. The spectral energy distribution corresponds to a Fock-Breit-Wigner (FBW) function, centered at w_0 and having a line breadth equal to the damping constant γ . Resonance is present even in the absence of external forces (transient oscillations). In such case the energy decreases exponentially with the time so that the damping constant γ is a measure of the lifetime of the oscillation

$\tau = 1/\gamma$. Similar phenomena occur for the electromagnetic radiation. In this context, the effects of radiative radiation can be approximated by considering the radiative reaction force \vec{F}_{rad} as a friction force which damps the oscillations of the electric field. Thus, the concept of resonance studied in classical mechanics is easily extended to the Maxwell's electromagnetic theory. The model also applies in vibrating elastic bodies, provided that the displacement is now a measure of the degree of excitation of the appropriate vibrational mode of the sample. *Acoustic resonances* are then obtained when the elastic bodies vibrate in such a way that standing waves are set up (Some interesting papers dealing with diverse kinds of resonances in metals can be consulted in [42]). Since the profile of atomic phenomena involving a high number of quanta of excitation can be analyzed in the context of classical mechanics, cyclotron and electron spin resonances can be studied, in a first approach, in terms of the above model (see, e.g. the paper by A.S. Nowick in [42], pp 1-44, and references quoted therein). The quantum approach to the problem of spinning charged particles showing magnetic resonance is discussed in conventional books on quantum mechanics like the one of Cohen-Tannoudji et. al. [43].

We have also shown that the resonance phenomenon occurs in quantum decaying systems. According with the Fock's approach, the corresponding law of decay depends only on the energy distribution function $\omega(E)$ which is meromorphic and acquires the form of a FBW, bell-shaped curve. The introduction of $\epsilon = E - i\Gamma/2$, a complex eigenvalue of the energy, is then required in analyzing the resonances which, in turn, are identified with the decaying states of the system. The inverse of the lifetime is then in correspondence with $\Gamma/2$. In a simple model, the related exponential decreasing probability can be justified by introducing a complex potential $U = U_R + U_I$, the imaginary part of which is the constant $-\Gamma/2$. Thus, U_I works like a sink of probability waves. The situation resembles the absorption of electromagnetic waves by a medium with complex refractive index so that $U = U_R + U_I$ is called an optical potential in nuclear physics. The treatment of complex energies in quantum mechanics includes non-square integrable Gamow-Siegert functions which are outside of the Hilbert spaces. In this sense, the complex-scaling method is useful to 'regularize' the problem by complex-rotating positions x and wavenumbers k . As a consequence, bounded and scattering states maintain without changes after the rotation while the Gamow-Siegert functions become square-integrable. Another important aspect of the method is that the positive real axis of the complex energy plane is clockwise rotated by an angle 2θ , so that resonant energies are exposed by the cuts of the corresponding Riemann surface. The method, however, also produces complex potentials. That is, the Gamow-Siegert functions are square-integrable solutions of a non-Hermitian Hamiltonian belonging to complex eigenvalues. Similar results are obtained by deforming the initial potential in terms of a Darboux transformation defined by a Gamow-Siegert function. In this sense, both of the above approaches could be applied in the studying of quantum resonances. A detailed analysis of the connection between the complex-scaling method and the Darboux-Gamow transformation is in progress.

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